

Table 1. Exemplary Nanotag Elements

Molecules	Vender	<i>MW</i> <i>g/mol</i>	Distinguishable Features
Fullerenes			
C60	BuckyUSA	720.6	size, shape, low density
C70	BuckyUSA	840.7	size, shape, low density
C84	BuckyUSA	1008.9	size, shape, low density
Metal Center Fullerenes			
C60La	BuckyUSA	859.5	size, shape, high electron density & charge
C84La	BuckyUSA	1147.8	size, shape, high electron density & charge
C60Er	BuckyUSA	887.5	size, shape, high electron density & charge
C84Er	BuckyUSA	1176.8	size, shape, high electron density & charge
Fullerene Oxides			
C60-O	BuckyUSA	736	size, shape, low density
C70-O	BuckyUSA	856	size, shape, low density
Bifunctional Fullerenes			
O-C60-O	BuckyUSA	752	size, shape, low density
O-C70-O	BuckyUSA	872	size, shape, low density
P.O.S.S. Polyhedral oligomeric silsesquioxane	Hybrid Plastics	800-1600	800-1600
Octakis pentacyclo octasiloxane hydrate	Aldrich	1137	Size, shape, charge (-)
OctaAmmonium POSS	Hybrid Plastics		Size, shape, charge (+)
OctaIsobutyl POSS	Hybrid Plastics		size, shape
OctaMethyl POSS	Hybrid Plastics		size, shape
Octa TmA POSS	Hybrid Plastics		size, shape, density

Table 1 (continued)

Organometallics			
Metal Centers include:Cr, Fe, Al, B, Co, Ni, Zr, Cu, Mg, Zn and Ru. Organic moieties include any functionalizable structure including, sepulcrates, bipyridines, porphrines, corrins, EDTA, biphenyl, benzene, phthalocyanine, hematoporphyrin, heme, naphthalocyanine, phthalocyanine, Cyclopentadiene, Indene, Fluorene, Benzoindene, 4-Fluorophenyl, 4-Methoxypheny, Tris(4-chlorophenyl) and others	Aldrich, Acros, Boulder Scientific		Metal centers have different size of outer orbital, density, charge distribution, and redox states. The organic moieties impart size, shape and density characteristics.
Cu II trifluoroacetyl acetate	Aldrich		
Cu II phthalocyanine	Aldrich		
Co II phthalocyanine	Aldrich		
Fe II phthalocyanine	Aldrich		
Zn II phthalocyanine	Aldrich		
Ni II phthalocyanine	Aldrich		
Mg II phthalocyanine	Aldrich		
Co II 2-3 naphthalocyanine	Aldrich		
1,1'-Ferrocenedicarboxylic acid	Aldrich	274.06	
Co III sepulcrate trichloride	Aldrich		
Cu II 2-pyrazinecarboxylate	Aldrich		
Nano-crystal particle (Ag), NHS esters	Nanoprobes		

TABLE 2. Potential Subunits for Backbone Mediated Synthesis

Candidate	Monofunctionalized	Attachment to subunit
C60	C60COOH	Lysine
C70	C70COOH	Lysine
La Buckey	LA Bucky COOH	Lysine
C60	C60COOH	Ethyl amino Thymidine
C70	C70COOH	Ethyl amino Thymidine
La Buckey	LA Bucky COOH	Ethyl amino Thymidine
(NH ₂) ₈ POSS	NA	Glutamic or aspartic acid
Metal Phalocyanonine	COOH	Lysine or NH ₂ -Thymidine
Metal Phalocyanonine	NH ₂	Glutamic or aspartic acid

Table 3. Exemplary Subunits for Polymer Decoration

Tag Element	Mono-functionalized	Attachment to polymer subunit	Polymer sequence
C60	C60COOH	Lysine	NH ₂ -(Gly-Gly-Gly-Lys) ₈ -COOH
C60	C60COOH	Lysine	NH ₂ -(A-A-A-A-A-A-K) ₇ -COOH
C70	C70COOH	Lysine	NH ₂ -(Gly-Gly-Gly-Lys) ₈ -COOH
C70	C70COOH	Lysine	NH ₂ -(A-A-A-A-A-A-K) ₇ -COOH
La Buckey	LA Bucky COOH	Lysine	NH ₂ -(Gly-Gly-Gly-Lys) ₈ -COOH
La Buckey	LA Bucky COOH	Lysine	NH ₂ -(A-A-A-A-A-A-K) ₇ -COOH
C60	C60COOH	Ethyl amino Thymidine (X)	5'-(T-X)10-3'
C60	C60COOH	Ethyl amino Thymidine (X)	5'-(X-Q) where Q is 12 atom spacer
C70	C70COOH	Ethyl amino Thymidine (X)	5'-(T-X)10-3'
C70	C70COOH	Ethyl amino Thymidine (X)	5'-(X-Q) where Q is 12 atom spacer
La Buckey	LA Bucky COOH	Ethyl amino Thymidine (X)	5'-(T-X)10-3'
La Buckey	LA Bucky COOH	Ethyl amino Thymidine (X)	5'-(X-Q) where Q is 12 atom spacer
(NH ₂) ₈ POSS	NA	Glutamic or aspartic acid	NH ₂ -(Gly-Gly-Gly-Glu) ₈ -COOH
(NH ₂) ₈ POSS	NA	Glutamic or aspartic acid	NH ₂ -(A-A-A-A-A-E) ₇ -COOH
(NH ₂) ₈ POSS	NA	T carboxylate analog (Y)	5'-(T-Y)10-3'
Metal Phalocyanine	COOH	Lysine	NH ₂ -(A-A-A-A-A-A-K) ₇ -COOH
Metal Phalocyanine	COOH	Lysine	NH ₂ -(Gly-Gly-Gly-Lys) ₈ -COOH

Table 4. Exemplary Subunits for Direct Polymer Imaging

Subunit	Polymer
Lysine (K)	(A ₆ -K) ₈ or (AAKAAAK) ₄ or KKKKKKKK
Glutamic acid (E)	(A ₆ -E) ₈ or (AAEAAAE) ₄ or EEEEEEE
E and K	(AAKAAAE) ₄
Br-T (Br)	T-Br-T-Br-TTT-Br-TTT-Br-Br-T
NH ₂ -T (N)	T-N-T-N-TTT-N-TTT-N-N-T
Br and N	T-Br-T-N-T-Br-Br-TTT-N-N-Br-T
Phosphate and spacers	TTT-3-9-3-3-9-9-3-9